Detection and identification of deep levels in n-GaN

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Deep levels in n-GaN have become prime suspects in limiting the behavior of GaN-based FET's, among other devices. In this paper the electronic and optical properties of deep levels present throughout the entire bandgap in unintentionally doped n-GaN are investigated by means of both deep level optical spectroscopy (DLOS) and deep level transient spectroscopy (DLTS). Hydrogenation, secondary ion mass spectroscopy (SIMS) and electron irradiation are used to investigate possible physical sources for these traps. While H incorporation is already known to play an important role in acceptor passivation in GaN, its effect on deep level properties is still almost unknown, and is expected to be a significant issue as GaN devices continue to evolve. Thus, post-growth RF plasma hydrogenation is used to directly evaluate the impact of H incorporation on the properties of deep levels. The interaction of H with these traps also aids in the identification of the defects responsible for the levels. These studies are complemented by results from electron irradiation on n-GaN which may help identify the point defects responsible for the levels found within this material.

Hydrogenation has a dramatic and non-uniform effect on deep levels within in MOCVD-grown n-GaN, differentially passivating some of the traps. Two types of behaviors are observed. First, two electron traps found at E_c - E_t =0.62 and 1.35 eV show strong H-passivation effects with their concentrations decreasing by a factor of ~30 and ~14, respectively (Figs. 1 and 2). The 0.62 eV trap concentration has been previously reported to track the residual Mg concentration measured by SIMS in n-GaN. This result taken together with the strong effect of H-incorporation strongly suggests that the passivation of the 0.62 eV level is consistent with Mg-H complex generation. These results may indicate that while shallow substitutional Mg acceptors (Mg_{Ga}) are known to react with H to create Mg-N-H complexes, Mg impurities may be incorporating at other lattice sites or complexing with other defects (possibly dislocations) that can also react with H. The 1.35 eV level has the closest energy to midgap of all the traps observed present and is thus potentially an efficient recombination-generation center that may impact n-GaN FET's. However, its physical origin is still unknown. Second, a band of closely spaced hole traps is observed at E_c - E_t =2.64 to 2.80 eV, which after hydrogenation narrows to E_c - E_t =2.74 to 2.80 eV, but its concentration remains constant (Fig. 2). This shift is better observed in the photocapacitance transient analysis not shown here for the sake of brevity. This band of states is most likely related to the yellow PL band, and shows a similar energy to reported calculations of deep levels produced by V_{Ga}^{3} and V_{Ga} - H_n complexes. Moreover, such calculations have shown that the hydrogenation of V_{Ga}^{3} to form $(V_{Ga}$ - $H_2)^{2}$ and $(V_{Ga}$ - $H_2)^{2}$ complexes each shift the level energy by ~0.1 eV closer to the valence band correlating with the 2.64 to 2.74 eV shift shown in Fig. 2. Thus, the E_c - E_t =2.64, 2.74 and 2.80 eV levels are assigned to V_{Ga}^{3} , $(V_{Ga}-H)^{2}$ and $(V_{Ga}-H_{2})^{2}$, respectively. Prior to hydrogenation the 2.74 eV threshold is probably present but likely obscured by the strong signal from the 2.64 eV level (Figs. 2), while the 2.80 eV level can be observed indicating the existence of $(V_{Ga}-H_2)^2$ complexes in the as-grown material. After hydrogenation, the 2.64 eV threshold is no longer observed due to the hydrogenation of V_{Ga}^3 which forms $(V_{Ga}-H)^2$ and $(V_{Ga}-H_2)^2$ consistent with their lower formation energies. We also conclude that post-growth hydrogenation of n-GaN has a small effect on the acceptor levels likely involved in the yellow PL emission. Finally, a hole trap found at E_c - E_r =3.22 eV is unaffected by H incorporation. This level is likely related to background acceptors found in MOCVD n-GaN, such as Mg or C. However, Mg acceptors are known to become strongly passivated by H. Thus Mg is most likely not related to the 3.22 eV hole trap, while C is not ruled out as the physical source. Further comparison of these results to n-GaN grown by MBE and in a Mg-free MOCVD reactor is ongoing and will be used to clarify the role of Mg, C and other impurities in the deep level generation.

Electron irradiation is used to generate point defects in MOCVD-grown n-GaN which allows the identification of the origin of some of the traps present in this material. Samples with low trap concentrations were

used for this study to allow the observation of induced defects in small concentrations. Preliminary results from electron irradiation with 1 MeV electrons under a fluence of 5×10^{15} cm⁻² show a distinct new feature: the DLOS spectrum shows a new threshold at ~2.80 eV (Fig. 3). This threshold correlates well with that observed in Fig. 2 and discussed above, and substantiates the role of point defects such as V_{Ga}^{3} in the formation of the 2.64 to 2.80 eV hole band. Moreover, other reports have associated V_{Ga}^{3} defects with the yellow PL band by means of positron annihilation spectroscopy. All these results taken together are a good indication that the 2.64 to 2.80 eV trap band is directly involved in the yellow PL emission in n-GaN. The origin of the defects induced by e-irradiation and its correlation to the deep level spectra of n-GaN grown both by MOCVD and MBE will also be addressed.

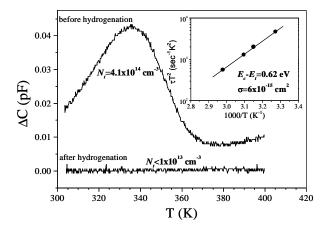


Fig. 1: Effect of hydrogenation on the DLTS spectra of n-GaN. The E_c - E_r =0.62 eV level concentration decreases by at least a factor of 30. Spectra shown for a rate window of 200 s⁻¹. The inset shows the Arrhenius behavior of this trap prior to hydrogenation.

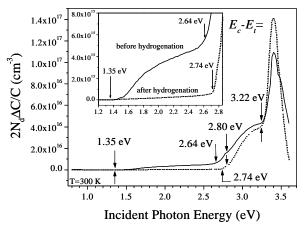


Fig. 2: a) Steady state photocapacitance spectra from n-GaN prior (solid line) and after hydrogenation (dashed line) measured at T=300 K. The concentration of a trap is proportional to the step it creates in the spectrum. b) Magnified view of the photocapacitance spectra where the strong effect of hydrogenation on the concentration of the 1.35 eV trap together with the 2.64 to 2.74 eV shift can be observed.

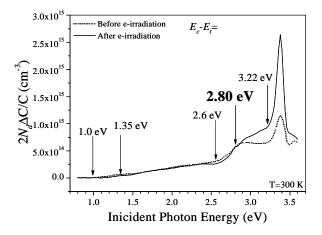


Fig. 3: Steady state photocapacitance spectra from n-GaN prior (dashed line) and after electron irradiation (solid line) measured at T=300 K. A new threshold at E_c - E_c =2.80 eV can be observed as a result of e-irradiation.